

=> s gambogat?

L1 5 GAMBOGAT?

=> d 11 105

5 ANSWERS ARE AVAILABLE. SPECIFIED ANSWER NUMBER EXCEEDS ANSWER SET SIZE

The answer numbers requested are not in the answer set.

ENTER ANSWER NUMBER OR RANGE (1):1-5

L1 ANSWER 1 OF 5 REGISTRY COPYRIGHT 2009 ACS on STN

RN 857500-90-4 REGISTRY

ED Entered STN: 28 Jul 2005

CN 2-Butenoic acid, 2-methyl-4-[(1R,3aS,5S,11R,14aS)-3a,4,5,7-tetrahydro-8-hydroxy-3,3,11-trimethyl-13-(3-methyl-2-buten-1-yl)-11-(4-methyl-3-penten-1-yl)-7,15-dioxo-1,5-methano-1H,3H,11H-furo[3,4-g]pyrano[3,2-b]xanthen-1-yl]-, 2-(dimethylamino)ethyl ester, (2Z)- (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 2-Butenoic acid, 2-methyl-4-[(1R,3aS,5S,11R,14aS)-3a,4,5,7-tetrahydro-8-hydroxy-3,3,11-trimethyl-13-(3-methyl-2-butenyl)-11-(4-methyl-3-pentenyl)-7,15-dioxo-1,5-methano-1H,3H,11H-furo[3,4-g]pyrano[3,2-b]xanthen-1-yl]-, 2-(dimethylamino)ethyl ester, (2Z)- (9CI)

OTHER NAMES:

CN 2-(Dimethylamino)ethyl gambogate

FS STEREOSEARCH

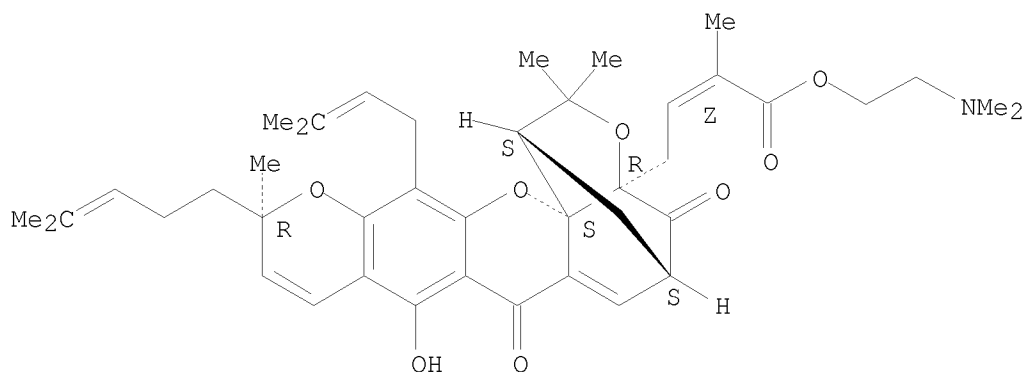
MF C42 H53 N O8

SR CA

LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER, USPATFULL

Absolute stereochemistry.

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L1 ANSWER 2 OF 5 REGISTRY COPYRIGHT 2009 ACS on STN

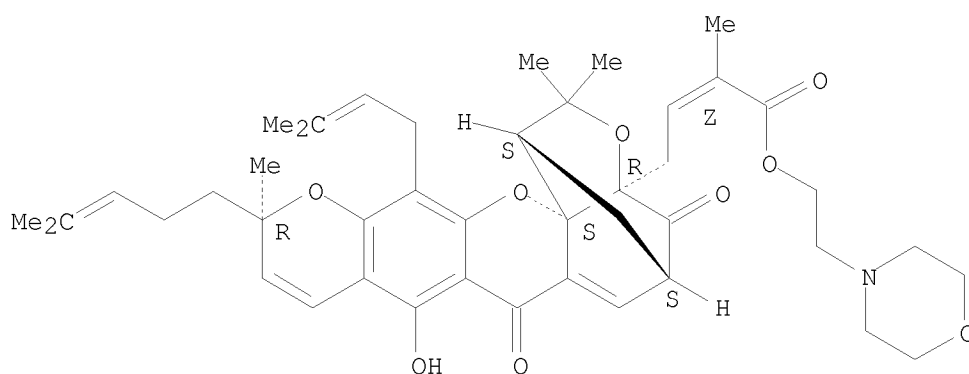
RN 857500-60-8 REGISTRY

ED Entered STN: 28 Jul 2005

CN 2-Butenoic acid, 2-methyl-4-[(1R,3aS,5S,11R,14aS)-3a,4,5,7-tetrahydro-8-hydroxy-3,3,11-trimethyl-13-(3-methyl-2-buten-1-yl)-11-(4-methyl-3-penten-1-yl)-7,15-dioxo-1,5-methano-1H,3H,11H-furo[3,4-g]pyrano[3,2-b]xanthen-1-

yl]-, 2-(4-morpholinyl)ethyl ester, (2Z)- (CA INDEX NAME)
 OTHER CA INDEX NAMES:
 CN 2-Butenoic acid, 2-methyl-4-[(1R,3aS,5S,11R,14aS)-3a,4,5,7-tetrahydro-8-hydroxy-3,3,11-trimethyl-13-(3-methyl-2-butenyl)-11-(4-methyl-3-pentenyl)-7,15-dioxo-1,5-methano-1H,3H,11H-furo[3,4-g]pyrano[3,2-b]xanthen-1-yl]-, 2-(4-morpholinyl)ethyl ester, (2Z)- (9CI)
 OTHER NAMES:
 CN 2-(Morpholin-4-yl)ethyl gambogate
 FS STEREOSEARCH
 MF C44 H55 N O9
 SR CA
 LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER, USPATFULL

Absolute stereochemistry.
 Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

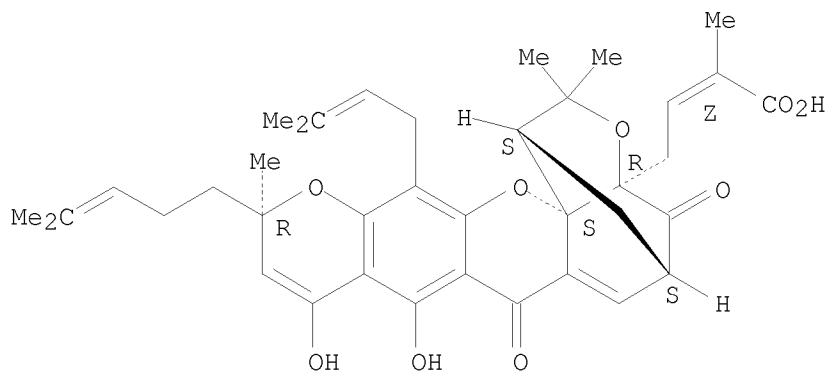
L1 ANSWER 3 OF 5 REGISTRY COPYRIGHT 2009 ACS on STN
 RN 849665-76-5 REGISTRY
 ED Entered STN: 03 May 2005
 CN Benzoic acid, 4-amino-, 2-(diethylamino)ethyl ester(2Z)-compd. with 2-methyl-4-[(1R,3aS,5S,11R,14aS)-3a,4,5,7-tetrahydro-8,9-dihydroxy-3,3,11-trimethyl-13-(3-methyl-2-butenyl)-11-(4-methyl-3-pentenyl)-7,15-dioxo-1,5-methano-1H,3H,11H-furo[3,4-g]pyrano[3,2-b]xanthen-1-yl]-2-butenoic acid (1:1) (CA INDEX NAME)
 OTHER CA INDEX NAMES:
 CN Benzoic acid, 4-amino-, 2-(diethylamino)ethyl ester, mono[(2Z)-2-methyl-4-[(1R,3aS,5S,11R,14aS)-3a,4,5,7-tetrahydro-8,9-dihydroxy-3,3,11-trimethyl-13-(3-methyl-2-butenyl)-11-(4-methyl-3-pentenyl)-7,15-dioxo-1,5-methano-1H,3H,11H-furo[3,4-g]pyrano[3,2-b]xanthen-1-yl]-2-butenoate] (9CI)
 OTHER NAMES:
 CN Procaine neogambogate
 FS STEREOSEARCH
 MF C38 H44 O9 . C13 H20 N2 O2
 SR CA
 LC STN Files: CA, CAPLUS, TOXCENTER

CM 1

CRN 849665-75-4

CMF C38 H44 O9

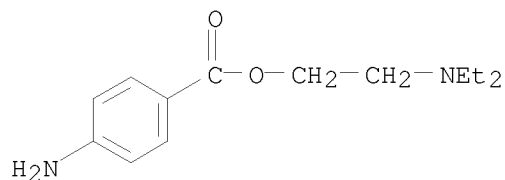
Absolute stereochemistry.
Double bond geometry as shown.



CM 2

CRN 59-46-1

CMF C13 H20 N2 O2

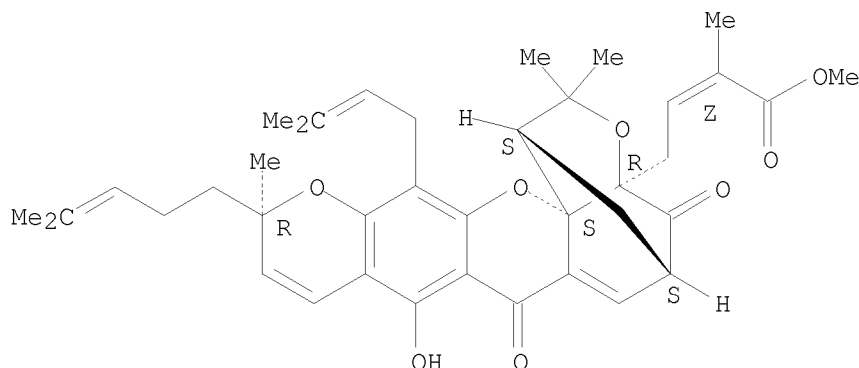


1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L1 ANSWER 4 OF 5 REGISTRY COPYRIGHT 2009 ACS on STN
RN 5914-82-9 REGISTRY
ED Entered STN: 16 Nov 1984
CN 2-Butenoic acid, 2-methyl-4-[(1R,3aS,5S,11R,14aS)-3a,4,5,7-tetrahydro-8-hydroxy-3,3,11-trimethyl-13-(3-methyl-2-buten-1-yl)-11-(4-methyl-3-penten-1-yl)-7,15-dioxo-1,5-methano-1H,3H,11H-furo[3,4-g]pyrano[3,2-b]xanthen-1-yl]-, methyl ester, (2Z)- (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 2-Butenoic acid, 2-methyl-4-[(1R,3aS,5S,11R,14aS)-3a,4,5,7-tetrahydro-8-hydroxy-3,3,11-trimethyl-13-(3-methyl-2-butenyl)-11-(4-methyl-3-pentenyl)-7,15-dioxo-1,5-methano-1H,3H,11H-furo[3,4-g]pyrano[3,2-b]xanthen-1-yl]-, methyl ester, (2Z)- (9CI)
CN Gambogic acid, methyl ester (7CI, 8CI)
OTHER NAMES:
CN Methyl gambogate
FS STEREOSEARCH
DR 47866-09-1
MF C39 H46 O8

CI COM
LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER, USPAT2, USPATFULL

Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

11 REFERENCES IN FILE CA (1907 TO DATE)
11 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L1 ANSWER 5 OF 5 REGISTRY COPYRIGHT 2009 ACS on STN
RN 2631-91-6 REGISTRY
ED Entered STN: 16 Nov 1984
CN 2-Butenoic acid, 2-methyl-4-[(1R,3aS,5S,11R,14aS)-3a,4,5,7-tetrahydro-8-hydroxy-3,3,11-trimethyl-13-(3-methyl-2-butenyl)-11-(4-methyl-3-pentenyl)-7,15-dioxo-1,5-methano-1H,3H,11H-furo[3,4-g]pyrano[3,2-b]xanthen-1-yl]-, (2Z)-, compd. with pyridine (1:1) (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 1,5-Methano-1H,3H,11H-furo[3,4-g]pyrano[3,2-b]xanthene-1-crotonic acid, 3a,4,5,7-tetrahydro-8-hydroxy- α ,3,3,11-tetramethyl-13-(3-methyl-2-butenyl)-11-(4-methyl-3-pentenyl)-7,15-dioxo-, (Z)-, compd. with pyridine (1:1) (8CI)

CN Gambogic acid, compd. with pyridine (7CI)

CN Pyridine, compd. with gambogic acid (1:1)

OTHER NAMES:

CN Pyridinium gambogate

FS STEREOSEARCH

MF C38 H44 O8 . C5 H5 N

LC STN Files: CA, CAPLUS, CASREACT, IMSRESEARCH, MRCK*, TOXCENTER, USPAT2, USPATFULL

(*File contains numerically searchable property data)

CM 1

CRN 2752-65-0

CMF C38 H44 O8

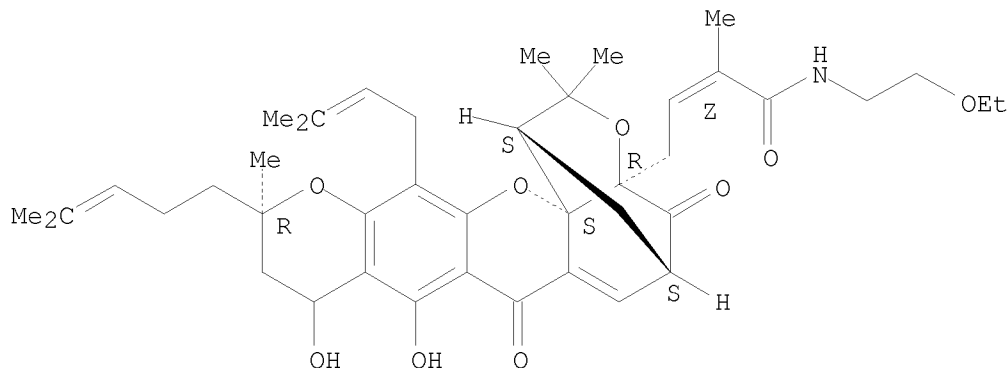
Absolute stereochemistry.
Double bond geometry as shown.

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L4      ANSWER 1 OF 5  REGISTRY  COPYRIGHT 2009 ACS  on STN
RN      905560-79-4   REGISTRY
ED      Entered STN:   31 Aug 2006
CN      2-Butenamide, N-(2-ethoxyethyl)-4-[(1R,3aS,5S,11R,14aS)-3a,4,5,7,10,11-
        hexahydro-8,9-dihydroxy-3,3,11-trimethyl-13-(3-methyl-2-buten-1-yl)-11-(4-
        methyl-3-penten-1-yl)-7,15-dioxo-1,5-methano-1H,3H,9H-furo[3,4-
        g]pyrano[3,2-b]xanthen-1-yl]-2-methyl-, (2Z)- (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN      2-Butenamide, N-(2-ethoxyethyl)-4-[(1R,3aS,5S,11R,14aS)-3a,4,5,7,10,11-
        hexahydro-8,9-dihydroxy-3,3,11-trimethyl-13-(3-methyl-2-butenyl)-11-(4-
        methyl-3-pentenyl)-7,15-dioxo-1,5-methano-1H,3H,9H-furo[3,4-g]pyrano[3,2-
        b]xanthen-1-yl]-2-methyl-, (2Z)- (9CI)
OTHER NAMES:
CN      N-(2-Ethoxyethyl)neogambogamide
CN      NG-18
FS      STEREOSEARCH
MF      C42 H55 N O9
SR      CA
LC      STN Files:    CA, CAPLUS, TOXCENTER

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Absolute stereochemistry.
 Double bond geometry as shown.
 Currently available stereo shown.

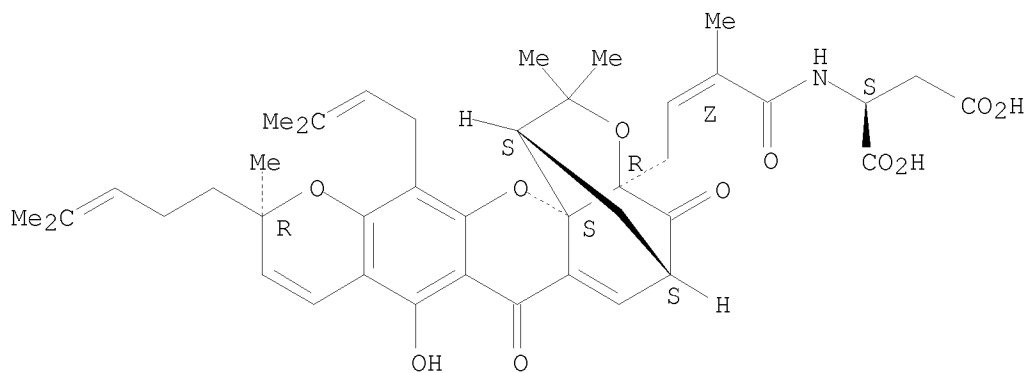


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
 2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L4 ANSWER 2 OF 5 REGISTRY COPYRIGHT 2009 ACS on STN
 RN 857501-29-2 REGISTRY
 ED Entered STN: 28 Jul 2005
 CN L-Aspartic acid, N-[(2Z)-2-methyl-1-oxo-4-[(1R,3aS,5S,11R,14aS)-3a,4,5,7-tetrahydro-8-hydroxy-3,3,11-trimethyl-13-(3-methyl-2-buten-1-yl)-11-(4-methyl-3-penten-1-yl)-7,15-dioxo-1,5-methano-1H,3H,11H-furo[3,4-g]pyrano[3,2-b]xanthen-1-yl]-2-buten-1-yl]- (CA INDEX NAME)
 OTHER CA INDEX NAMES:
 CN L-Aspartic acid, N-[(2Z)-2-methyl-1-oxo-4-[(1R,3aS,5S,11R,14aS)-3a,4,5,7-tetrahydro-8-hydroxy-3,3,11-trimethyl-13-(3-methyl-2-butenyl)-11-(4-methyl-3-pentenyl)-7,15-dioxo-1,5-methano-1H,3H,11H-furo[3,4-g]pyrano[3,2-b]xanthen-1-yl]-2-butenyl]- (9CI)
 OTHER NAMES:
 CN N-[(S)-1,2-Dicarboxyethyl]gambogamide
 FS STEREOSEARCH
 MF C42 H49 N O11
 SR CA
 LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER, USPATFULL

Absolute stereochemistry.
 Double bond geometry as shown.



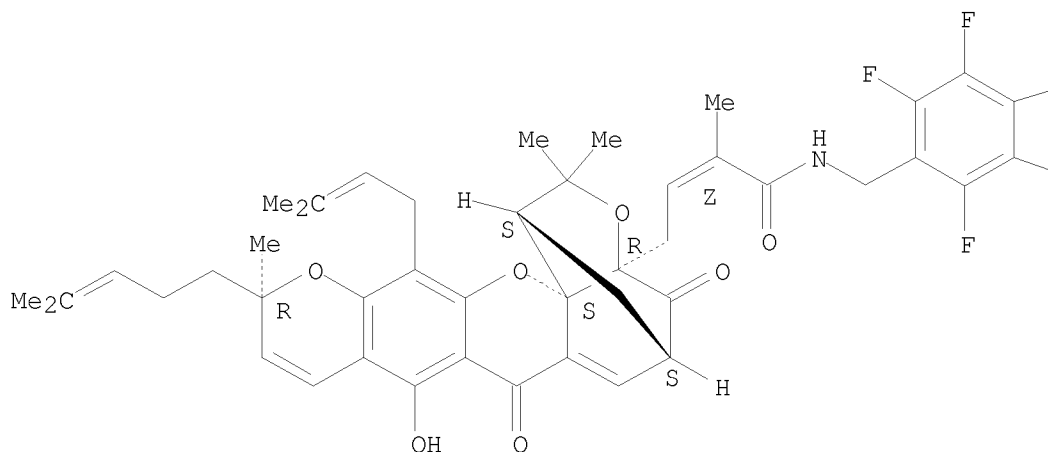
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L4 ANSWER 3 OF 5 REGISTRY COPYRIGHT 2009 ACS on STN
RN 857501-27-0 REGISTRY
ED Entered STN: 28 Jul 2005
CN 2-Butenamide, N-[(4-azido-2,3,5,6-tetrafluorophenyl)methyl]-2-methyl-4-[(1R,3aS,5S,11R,14aS)-3a,4,5,7-tetrahydro-8-hydroxy-3,3,11-trimethyl-13-(3-methyl-2-buten-1-yl)-11-(4-methyl-3-penten-1-yl)-7,15-dioxo-1,5-methano-1H,3H,11H-furo[3,4-g]pyrano[3,2-b]xanthen-1-yl]-, (2Z)- (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 2-Butenamide, N-[(4-azido-2,3,5,6-tetrafluorophenyl)methyl]-2-methyl-4-[(1R,3aS,5S,11R,14aS)-3a,4,5,7-tetrahydro-8-hydroxy-3,3,11-trimethyl-13-(3-methyl-2-butenyl)-11-(4-methyl-3-pentenyl)-7,15-dioxo-1,5-methano-1H,3H,11H-furo[3,4-g]pyrano[3,2-b]xanthen-1-yl]-, (2Z)- (9CI)
OTHER NAMES:
CN N-(4-Azido-2,3,5,6-tetrafluorobenzyl)gambogamide
FS STEREOSEARCH
MF C45 H46 F4 N4 O7
SR CA
LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER, USPATFULL

Absolute stereochemistry.
Double bond geometry as shown.

PAGE 1-A



N3

F

1 REFERENCES IN FILE CA (1907 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L4 ANSWER 4 OF 5 REGISTRY COPYRIGHT 2009 ACS on STN

RN 857500-92-6 REGISTRY

ED Entered STN: 28 Jul 2005

CN 2-Butenamide, 2-methyl-N-[3-(4-morpholinyl)propyl]-4-[(1R,3aS,5S,11R,14aS)-3a,4,5,7-tetrahydro-8-hydroxy-3,3,11-trimethyl-13-(3-methyl-2-buten-1-yl)-11-(4-methyl-3-penten-1-yl)-7,15-dioxo-1,5-methano-1H,3H,11H-furo[3,4-gl]pyrano[3,2-b]xanthen-1-yl]-, (2Z)- (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 2-Butenamide, 2-methyl-N-[3-(4-morpholinyl)propyl]-4-[(1R,3aS,5S,11R,14aS)-3a,4,5,7-tetrahydro-8-hydroxy-3,3,11-trimethyl-13-(3-methyl-2-butenyl)-11-(4-methyl-3-pentenyl)-7,15-dioxo-1,5-methano-1H,3H,11H-furo[3,4-gl]pyrano[3,2-b]xanthen-1-yl]-, (2Z)- (9CI)

OTHER NAMES:

CN N-[3-(Morpholin-4-yl)propyl]gambogamide

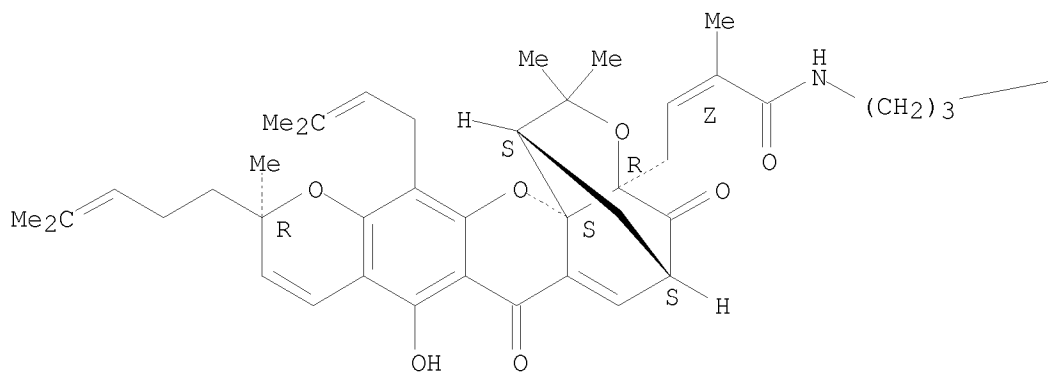
FS STEREOSEARCH

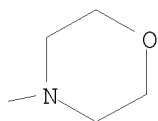
MF C45 H58 N2 O8

SR CA

LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER, USPATFULL

Absolute stereochemistry.
 Double bond geometry as shown.



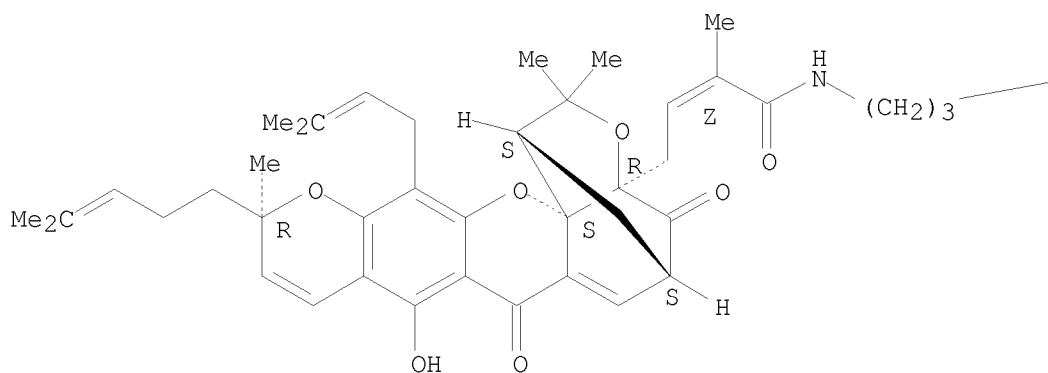


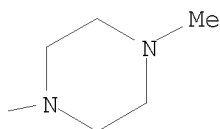
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L4 ANSWER 5 OF 5 REGISTRY COPYRIGHT 2009 ACS on STN
RN 857500-91-5 REGISTRY
ED Entered STN: 28 Jul 2005
CN 2-Butenamide, 2-methyl-N-[3-(4-methyl-1-piperazinyl)propyl]-4-
[(1R,3aS,5S,11R,14aS)-3a,4,5,7-tetrahydro-8-hydroxy-3,3,11-trimethyl-13-(3-
methyl-2-buten-1-yl)-11-(4-methyl-3-penten-1-yl)-7,15-dioxo-1,5-methano-
1H,3H,11H-furo[3,4-g]pyrano[3,2-b]xanthen-1-yl]-, (2Z)- (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 2-Butenamide, 2-methyl-N-[3-(4-methyl-1-piperazinyl)propyl]-4-
[(1R,3aS,5S,11R,14aS)-3a,4,5,7-tetrahydro-8-hydroxy-3,3,11-trimethyl-13-(3-
methyl-2-butenyl)-11-(4-methyl-3-pentenyl)-7,15-dioxo-1,5-methano-
1H,3H,11H-furo[3,4-g]pyrano[3,2-b]xanthen-1-yl]-, (2Z)- (9CI)
OTHER NAMES:
CN N-[3-(4-Methylpiperazin-1-yl)propyl]gambogamide
FS STEREOSEARCH
MF C46 H61 N3 O7
SR CA
LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER, USPATFULL

Absolute stereochemistry.
Double bond geometry as shown.





PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

> s l4

L5 3 L4

=> d l5 1-3 ibib abs hitstr

L5 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2007:1088055 CAPLUS <<LOGINID::20090326>>

DOCUMENT NUMBER: 149:323145

TITLE: Caspase-8 preferentially senses the apoptosis-inducing action of NG-18, a gambogic acid derivative, in human leukemia HL-60 cells

AUTHOR(S): Tao, Zhijian; Zhou, Yunlong; Lu, Jinjian; Duan, Wenhui; Qin, Yuxin; He, Xinxia; Lin, Liping; Ding, Jian

CORPORATE SOURCE: College of Chemistry and Life, Zhejiang Normal University, Jinhua Zhejiang, Peop. Rep. China

SOURCE: Cancer Biology & Therapy (2007), 6(5), 691-696
CODEN: CBTAAO; ISSN: 1538-4047

PUBLISHER: Landes Bioscience

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Gambogic acid (GA) is the major active ingredient of gamboge secreted from a Chinese traditional medicine *Garcinia hanburyi* possessing potent anti-tumor activity. N-(2-ethoxyethyl)neogambogamide (NG-18), a derivative of GA, also efficiently inhibits proliferation of cultured human tumor cells. The inhibition effect of NG-18 is associated with its ability to induce apoptosis. In the present study, NG-18 markedly induced leukemia HL-60 cells apoptosis, and the extrinsic and intrinsic apoptosis pathways were activated almost at the same time. NG-18-induced tumor cell apoptosis was associated with up-regulation of pro-apoptotic Bcl-2 family member Bax, and downregulation of anti-apoptotic protein Bcl-2. The NG-18-induced apoptosis was blocked completely by a pan-caspase inhibitor Z-VAD-FMK, indicating that caspases were functionally and actively involved in this process. The specific inhibition of caspase-8 activity using Z-IETD-FMK significantly blocked NG-18-induced apoptosis. In contrast, inhibition of other initiator caspases, caspase-2 or -9, using Z-VDVAD-FMK or Z-LEHD-FMK resp. had no effect on NG-18-induced apoptosis. Altogether, the authors' data demonstrated that NG-18-induced apoptosis was dependent on caspases and caspase-8 acted as a key executor in the event.

IT 905560-79-4, N-(2-Ethoxyethyl)neogambogamide

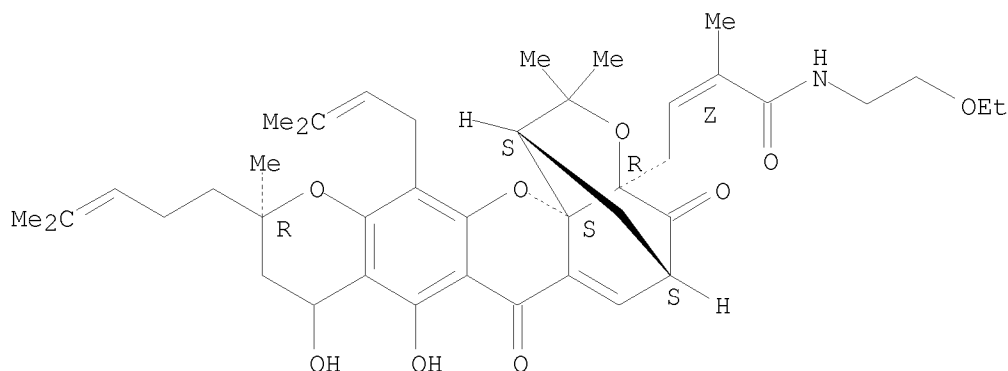
RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(NG-18; gambogic acid derivative N-(2-ethoxyethyl)neogambogamide showed anticancer activity, induced extrinsic and intrinsic apoptosis pathway preferentially mediated by caspase-8 in human leukemia cell)

RN 905560-79-4 CAPLUS

CN 2-Butenamide, N-(2-ethoxyethyl)-4-[(1R,3aS,5S,11R,14aS)-3a,4,5,7,10,11-hexahydro-8,9-dihydroxy-3,3,11-trimethyl-13-(3-methyl-2-buten-1-yl)-11-(4-methyl-3-penten-1-yl)-7,15-dioxo-1,5-methano-1H,3H,9H-furo[3,4-g]pyrano[3,2-b]xanthen-1-yl]-2-methyl-, (2Z)- (CA INDEX NAME)

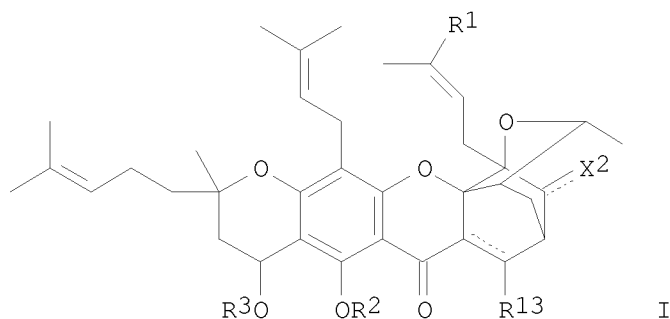
Absolute stereochemistry.
Double bond geometry as shown.
Currently available stereo shown.



REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2006:459169 CAPLUS <<LOGINID::20090326>>
DOCUMENT NUMBER: 145:230466
TITLE: Neogambogic acid derivatives used to treat cancer, and preparation thereof
INVENTOR(S): Duan, Wenhui; Zhou, Yunlong; Jiang, Hualiang; Ding, Jian; Luo, Xiaomin; Chen, Yi
PATENT ASSIGNEE(S): Shanghai Institute of Materia Medica, Chinese Academy of Sciences, Peop. Rep. China
SOURCE: Faming Zhuanli Shenqing Gongkai Shuomingshu, 37 pp. CODEN: CNXXEV
DOCUMENT TYPE: Patent
LANGUAGE: Chinese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CN 1715283	A	20060104	CN 2004-10025719	20040702
PRIORITY APPLN. INFO.:			CN 2004-10025719	20040702
OTHER SOURCE(S):	MARPAT	145:230466		
GI				



AB The title Gambogic acid derivs. have general formula I ($R_3 = H$, C1-10 alkyl-substituted or aryl-substituted acyl; $R_2 = H$, linear or branched C1-10 alkyl, C3-8 cycloalkyl, aryl or aryl substituted with C1-10 alkyl, heteroaryl, C1-10 alkyl-substituted or aryl-substituted acyl; $X_2 =$ carbonyl oxygen atom or hydroxyl; $R_{13} =$ linear or branched C1-10 alkyl, C3-8 cycloalkyl, linear or branched C2-10 alkenyl or C3-10 cycloalkenyl, Ph or C1-10 alkyl-substituted Ph, etc.; $R_1 = -COOR_4$ with R_4 being H, linear or branched C1-10 alkyl, alkyl with 1-3 substituting groups selected from oxyl, halogen, C1-10 alkyl, alkanoyloxyl, aryloxyl, etc., C3-8 cycloalkyls, alkyls substituted with 1-3 hetero atoms, arylalkyls, etc., or $-CONR_5R_6$ with R_5 and R_6 being H, linear or branched C-10 alkyls, alkyls substituted with 1-3 groups selected from hydroxyl, amino, C1-10 alkylamino, oxyl, halogens, etc., C3-8 cycloalkyls, C1-10 alkyls substituted with 1-3 heteroatoms, arylalkyls, etc.). The title preparation includes subjecting Neogambogic acid to condensation, etherification, reduction, and acylation to obtain compds. I, and carrying out addition with hydrogen peroxide to the C9 C10 bond of Neogambogic acid in the presence of a base, or carrying out 1,4-addition with organocopper reagent to the C9 C10 bond to obtain compound derivs. Title compds. can be applied in treating cancer.

IT 905560-79-4P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(synthesis of Neogambogic acid derivs. as antitumor agent)

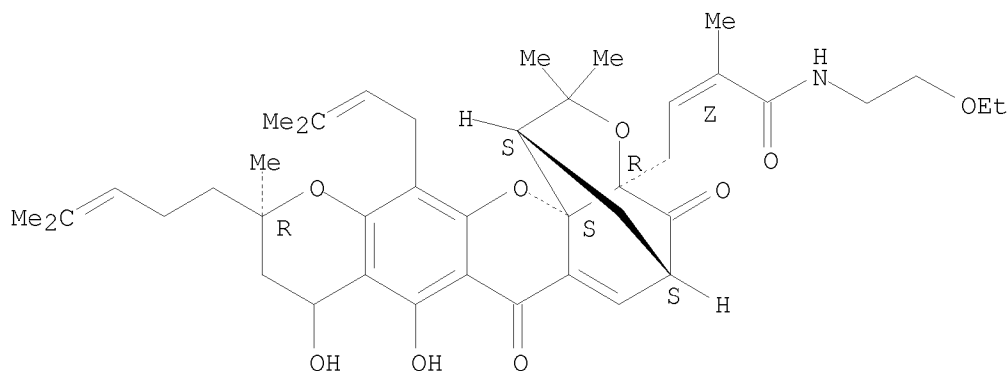
RN 905560-79-4 CAPLUS

CN 2-Butenamide, N-(2-ethoxyethyl)-4-[(1R,3aS,5S,11R,14aS)-3a,4,5,7,10,11-hexahydro-8,9-dihydroxy-3,3,11-trimethyl-13-(3-methyl-2-buten-1-yl)-11-(4-methyl-3-penten-1-yl)-7,15-dioxo-1,5-methano-1H,3H,9H-furo[3,4-g]pyrano[3,2-b]xanthen-1-yl]-2-methyl-, (2Z)- (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

Currently available stereo shown.



L5 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 2005:588556 CAPLUS <<LOGINID::20090326>>
 DOCUMENT NUMBER: 143:115395
 TITLE: Preparation of derivatives of gambogic acid and
 analogs as activators of caspases and inducers of
 apoptosis
 INVENTOR(S): Cai, Sui Xiong; Jiang, Songchun; Zhang, Han-Zhong
 PATENT ASSIGNEE(S): Cytovia, Inc., USA
 SOURCE: PCT Int. Appl., 51 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005060663	A2	20050707	WO 2004-US42292	20041217
WO 2005060663	A3	20051222		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, SM			
RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
US 20070093456	A1	20070426	US 2006-580263	20060525
PRIORITY APPLN. INFO.:			US 2003-530256P	P 20031218
			WO 2004-US42292	W 20041217
OTHER SOURCE(S):	CASREACT 143:115395			
GI				

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The present invention is directed to novel derivs. of gambogic acid (I) and analogs thereof. Thus, 2-(Dimethylamino)ethyl gambogate (II) was prepared from I via esterification with ClCH2CH2NMe2·HCl in the

presence of KI and Cs2CO4. The present invention also relates to the discovery that novel derivs. of gambogic acid are activators of caspases and inducers of apoptosis. Therefore, the activators of caspases and inducers of apoptosis of this invention can be used to induce cell death in a variety of clin. conditions in which uncontrolled growth and spread of abnormal cells occurs. The bioactivity of II was determined [caspase cascade activation EC50 = 676 nM vs. T-47D and EC50 = 1041 nM vs. DLD breast cancer cells; cell proliferation inhibition GI50 = 187 nM (vs. T-47D), GI50 = 173 nM (vs. DLD), GI50 = 101 nM (vs. MX-1), GI50 = 180 nM (vs. SW620), GI50 = 184 nM (vs. H1299), GI50 = 440 nM (vs. HEK293T), GI50 = 192 nM (vs. HEK293H)].

IT 857500-91-5P, N-[3-(4-Methylpiperazin-1-yl)propyl]gambogamide
 857500-92-6P, N-[3-(Morpholin-4-yl)propyl]gambogamide
 857501-27-0P, N-(4-Azido-2,3,5,6-tetrafluorobenzyl)gambogamide
 857501-29-2P, N-[(S)-1,2-Dicarboxyethyl]gambogamide

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

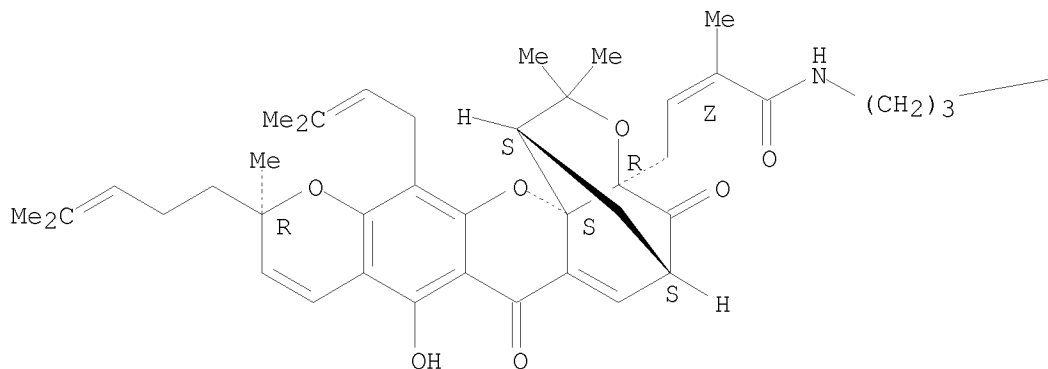
(preparation of derivs. of gambogic acid and analogs as activators of caspases and inducers of apoptosis)

RN 857500-91-5 CAPLUS

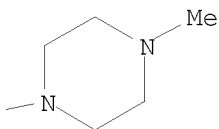
CN 2-Butenamide, 2-methyl-N-[3-(4-methyl-1-piperazinyl)propyl]-4-[(1R,3aS,5S,11R,14aS)-3a,4,5,7-tetrahydro-8-hydroxy-3,3,11-trimethyl-13-(3-methyl-2-buten-1-yl)-11-(4-methyl-3-penten-1-yl)-7,15-dioxo-1,5-methano-1H,3H,11H-furo[3,4-g]pyrano[3,2-b]xanthen-1-yl]-, (2Z)- (CA INDEX NAME)

Absolute stereochemistry.
 Double bond geometry as shown.

PAGE 1-A



PAGE 1-B



RN 857500-92-6 CAPLUS

CN 2-Butenamide, 2-methyl-N-[3-(4-morpholinyl)propyl]-4-[(1R,3aS,5S,11R,14aS)-3a,4,5,7-tetrahydro-8-hydroxy-3,3,11-trimethyl-13-(3-methyl-2-buten-1-yl)-

Absolute stereochemistry.
Double bond geometry as shown.

The chemical structure shows a complex polycyclic molecule, likely a steroid derivative. It features a central fused ring system with several substituents. On the left, a long alkyl chain is attached to a ring, with a methyl group (Me) and a hydroxyl group (OH) nearby. The central ring system includes a ketone group (C=O) and a hydroxyl group (OH). On the right, a side chain is attached, containing a methyl group (Me), a hydroxyl group (OH), and a long alkyl chain ending in a methyl group (Me). The structure is labeled with 'Me' for methyl, 'OH' for hydroxyl, and 'R' for a variable group. Stereochemistry is indicated with 'H' and 'S' labels.

CN1CCOCC1

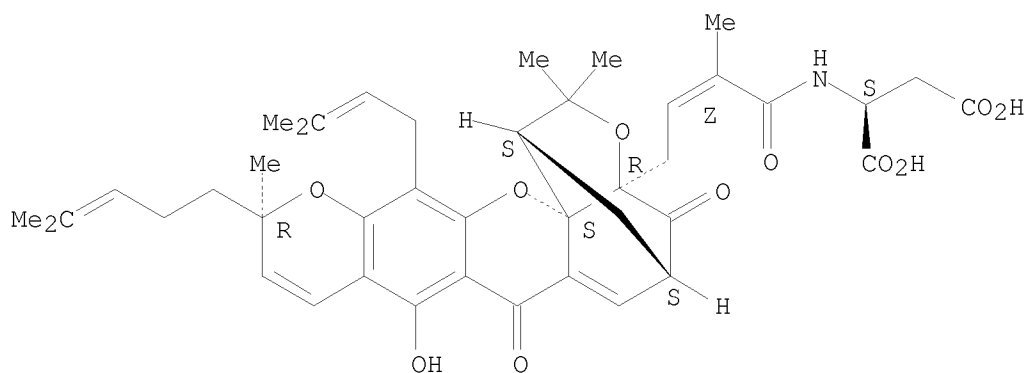
Absolute stereochemistry.
Double bond geometry as shown.

N3

F

RN 857501-29-2 CAPLUS
 CN L-Aspartic acid, N-[(2Z)-2-methyl-1-oxo-4-[(1R,3aS,5S,11R,14aS)-3a,4,5,7-tetrahydro-8-hydroxy-3,3,11-trimethyl-13-(3-methyl-2-buten-1-yl)-11-(4-methyl-3-penten-1-yl)-7,15-dioxo-1,5-methano-1H,3H,11H-furo[3,4-g]pyrano[3,2-b]xanthen-1-yl]-2-buten-1-yl]- (CA INDEX NAME)

Absolute stereochemistry.
 Double bond geometry as shown.



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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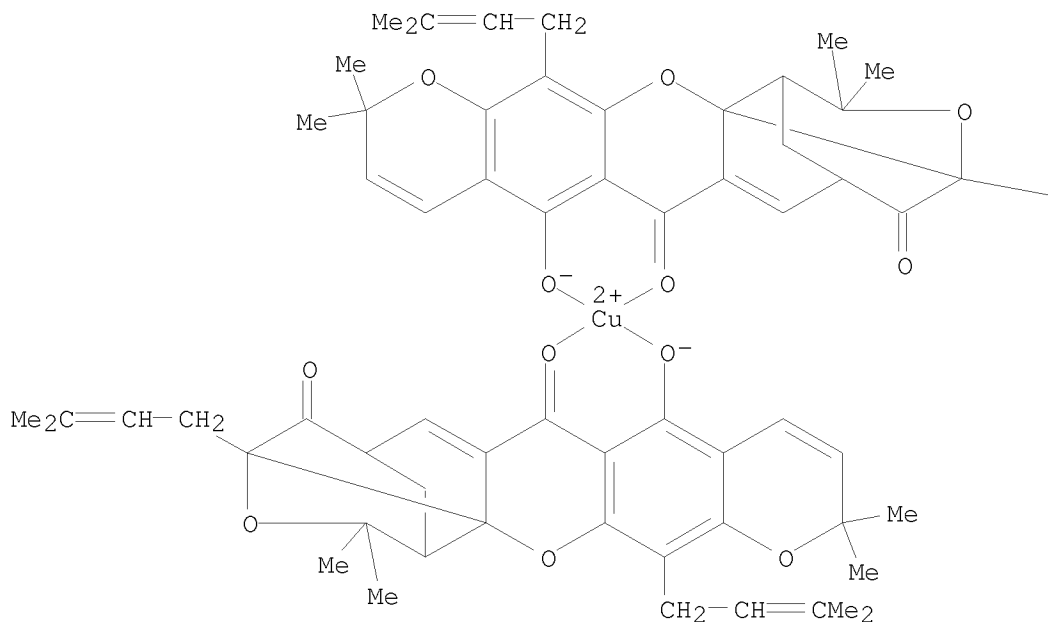
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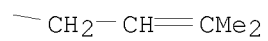
L6 1 MORELLINAT?

=> d 16

L6 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2009 ACS on STN
RN 14916-03-1 REGISTRY
ED Entered STN: 16 Nov 1984
CN Copper, bis(deoxymorellinato-07,08)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Morellin, deoxy-, Cu deriv. (7CI)
MF C66 H74 Cu O12
CI CCS
LC STN Files: CA, CAPLUS

PAGE 1-A





1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

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